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Maximum complexity distribution of a monodimensional ideal gas out of equilibrium

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Abstract

The maximum complexity momentum distribution for an isolated monodimensional ideal gas out of equilibrium is derived analytically. In a first approximation, it consists of a double non-overlapping Gaussian distribution. In good agreement with this result, the numerical simulations of a particular isolated monodimensional gas, which is abruptly pushed far from equilibrium, shows the maximum complexity distribution in the decay of the system toward equilibrium.

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1. INTRODUCTION

Boltzmann–Gibbs (BG) statistics works perfectly for classical systems in equilibrium under the action of short-range forces. But most systems in nature are out of equilibrium and there is no a priori reason why a particular phenomenon should behave according to a specific kind of statistics. If the system finally decays toward equilibrium, then the asymptotic long-time limit should be that of BG statistics.

Different kinds of statistics have been proposed to model different nonequilibrium situations. For instance, *non-extensive thermostatistics* is based on maximizing the Tsallis entropy [1] under different assumptions for calculating the expectation value of the energy. Power law distributions are obtained by fixing the total energy of the system in all the cases analyzed in Ref. [2]. Thus, in this scheme, the exponential distribution of BG statistics turns out to be a singularity that is recovered in the limit $q \to 1$, where q is called the index of non-extensivity. Although this type of statistics might seem a mathematical artifact without applications, several types of generalized stochastic dynamics have been recently constructed for which Tsallis statistics can be proved rigorously [3]. Also, it has been found useful in explaining many other physical phenomena [4, 5]. Another formalism to study out of equilibrium situations is *superstatistics*. Originally proposed by Beck and Cohen [6], it deals with nonequilibrium systems with a long-term stationary state that possess a spatio–temporally fluctuating intensive quantity. After averaging over the fluctuations one can obtain an infinite set of general statistics called superstatistics, which constitute a superposition of BG distributions. Tsallis statistics is a special case of such superstatistics, and, in particular, BG statistics is also recovered when $q \to 1$, where q is now a dynamical parameter with a certain physical interpretation. In general, complex nonequilibrium problems may require different types of superstatistics [6].

Although all these statistical techniques for modeling out of equilibrium situations are becoming a well established theory, as far as we know, there are no general laws telling us in what manner a system should relax towards equilibrium. The second law of thermodynamics claims that the average entropy or disorder must increase when an isolated system tends to equilibrium but no more insight is obtained from this postulate. In fact, this law in no way forbids local complexity from arising [7]. An inspiring example is life, which can continue to exist and replicate in an isolated system as long as internal resources last. It could then

be postulated that in an isolated system, besides an increase in entropy, the system will try to stay close to the maximum complexity state. This behavior was found in Ref. [8] for a particular system, the "tetrahedral" gas, when complexity is defined as in Ref. [9] (referred to in the literature as the LMC complexity). Furthermore, it was established that this isolated system relaxes towards equilibrium by approaching *the maximum complexity path.* This path is an attractive trajectory in the distribution space connecting all the maximum complexity distributions (see Ref. [8] for details).

In this paper, we perform the study of an isolated monodimensional ideal gas that is initially in equilibrium, receives a strong perturbation, and finally freely decays towards equilibrium. The one-particle momentum distribution is computationally calculated for each time during the relaxation process. It is found that this distribution coincides with the maximum LMC-complexity one-particle momentum distribution. Hence, the maximum complexity path in the space of one particle momentum distributions also seems to explain the statistical evolution of this system when it approaches equilibrium.

2. NUMERICAL SIMULATIONS OF A MONODIMENSIONAL GAS

In order to have a graphical picture of the processes involved, we start by describing the numerical simulations. The gas is initially, at time $t = 0$, in equilibrium. Its one particle momentum distribution is described by a Gaussian or Maxwell–Boltzmann function. At this point, two new extremely energetic particles are introduced into the gas, forcing the gas into a far from equilibrium state. The system is kept isolated from then on. It eventually relaxes again toward equilibrium showing asymptotically another Gaussian distribution. Most of the time, during this out of equilibrium process, the momentum distribution function is described to a first approximation by two Gaussian distributions. This double Gaussian distribution coincides with the analytically derived maximum complexity distribution, which will be derived later.

In more detail, and using arbitrary units from now on, the gas consisted of 10 000 pointlike particles colliding with each other elastically. The particles were positioned with alternating masses of 1 and 2 on regular intervals on a linear space 10 000 units long. The system has no boundaries, i.e., the last particle in this linear space was allowed to collide with the first one, in a way similar to a set of rods on a circular ring. Two distinct masses in the system were

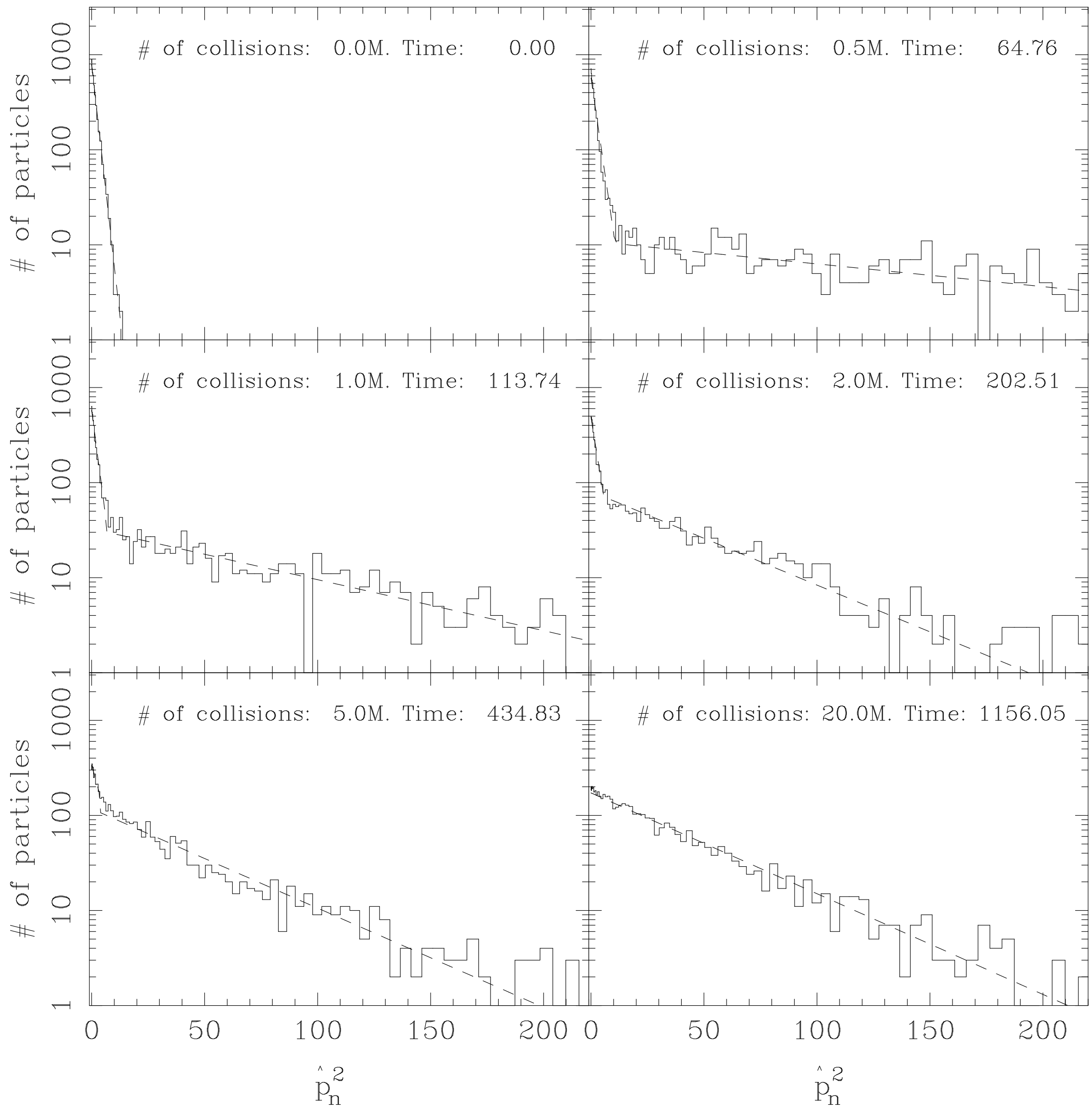

FIG. 1: Results of the numerical simulations of an isolated monodimensional ideal gas when it relaxes towards equilibrium (lower right) from an initial condition in which two very energetic particles are introduced into the gas in equilibrium (upper left). Histograms of the one-particle momentum distribution with a log vertical axis at various times are shown as solid lines. A double Gaussian fit, the maximum complexity distribution, is shown as dashed lines.

used because a monodimensional gas can thermalize only if its constituent particles have at least two different masses. Initially 9998 particles were given initial conditions following a Gaussian distribution with mean zero velocity and a mean energy of 1/2, giving a total mean energy for the system of nearly 5000. These particles where then allowed to undergo 20 million collisions in order for the system to reach the initial state of equilibrium, i.e., a Gaussian

distribution. After that, at time $t = 0$ two extremely energetic particles of mass 1 and 2 are introduced at two neighboring points, such that the total system has zero momentum and an energy of 150 000. The system then undergoes another 20 million collisions to reach again the equilibrium Gaussian distribution after a total elapsed time of $\Delta t = 1156.05$. We record the time evolution of the one-dimensional momentum distribution in Fig. 1, where the square of the generalized particle momentum is given by the variable $\hat{p}_i^2 \equiv p_i^2/m_i$, with p_i and m_i the momentum and mass of particle i. The theoretical maximum complexity distribution (derived below) for this system is approximated by two non-overlapping Gaussian distributions and is also fitted as dashed lines in Fig. 1. Let us remark that the system stays in this double Gaussian, the maximum complexity distribution, during a large part of its out of equilibrium phase. The two clearly visible slopes of Fig. 1 are related with the two different mean energies associated with both Gaussian distributions. As the system approaches equilibrium, both Gaussian distributions merge into one.

In Fig. 2 the momentum distribution is shown at a particular moment out of equilibrium (solid line). In this case a direct histogram of the momentum distribution is shown. The double gaussian or maximum complexity distribution is clearly seen. In this Figure, the complete gaussian distributions are shown for clarity (dashed lines), but the fit to the numerical simulated data has been done with non-overlaping Gaussian functions.

3. MAXIMUM COMPLEXITY DISTRIBUTION

We now sketch the analytical derivation of the microcanonical maximum complexity distribution for a system with a huge number of accessible states. In Ref. [8], the maximum complexity distribution for an isolated system with a discrete number of accessible states was derived. This type of distribution was found to be important in the path towards equilibrium for a particular isolated gas, the tetrahedral gas. When this system is out equilibrium it decays to equilibrium by approaching the trajectory formed by all the maximum complexity distributions and called the maximum complexity path. Finding these extremal distributions requires solving a variational problem. The *complexity* C (see Ref. [9]), is defined as

$$C = D \cdot H, \tag{1}$$

where the *disequilibium*, D, is defined as the distance to the microcanonical equilibrium

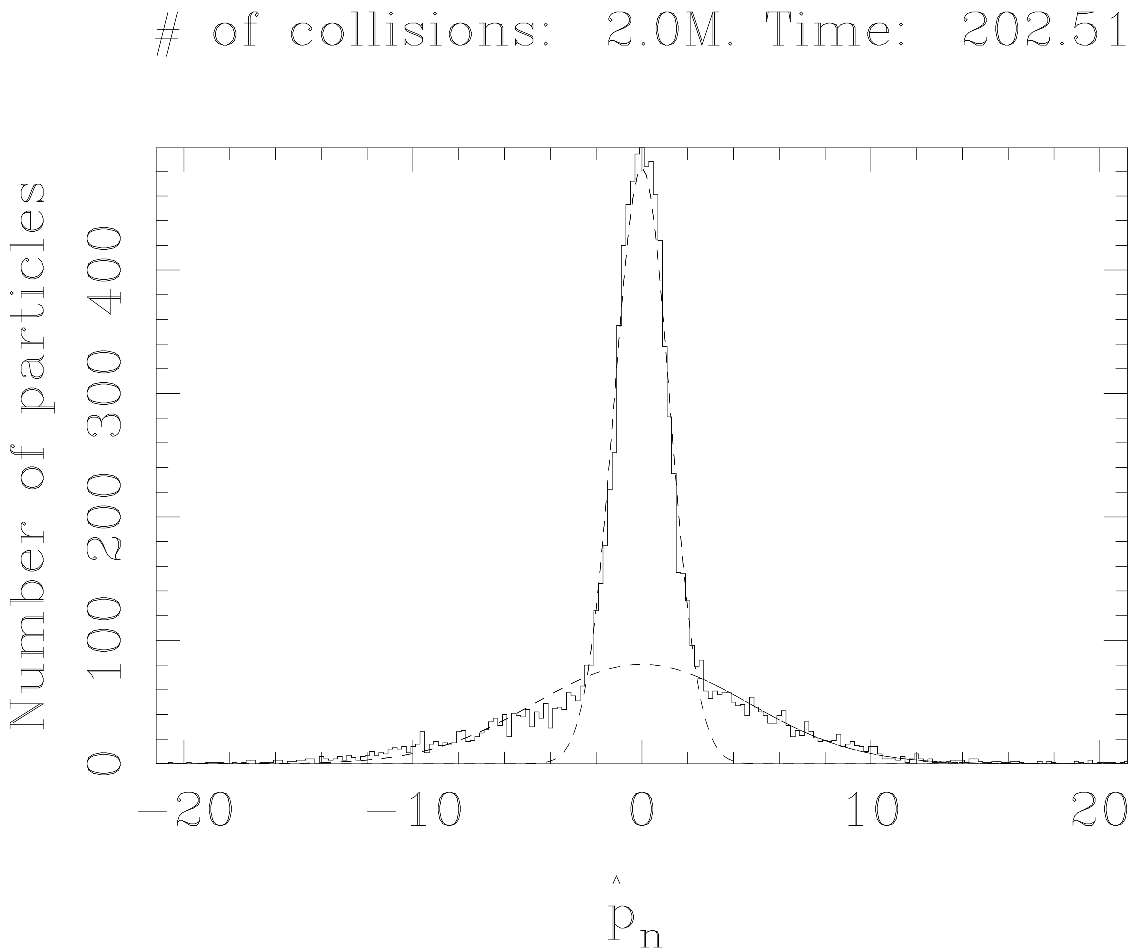

FIG. 2: Numerical simulations of an isolated monodimensional ideal gas as it relaxes to equilibirum at a particular time, 202.5 after 2 million collisions. The histogram of the one particle momentum distribution is shown as a solid line. The two fitted gaussian distributions, the maximum complexity distribution, are shown as dashed lines.

probability distribution, the equiprobability, and H is the *normalized entropy*,

$$D = \sum_{i=1}^{N} (f_i - 1/N)^2 \text{ and } H = -(1/\ln N) \sum_{i=1}^{N} f_i \ln f_i, \tag{2}$$

where N is the number of accessible states and f_i, with $i = 1, 2, \ldots, N$, are the probabilities of permanence that the system presents for the different discrete accessible states i. Thus, the microcanonical maximum complexity distribution can be derived by finding the maximum disequilibrium for a given entropy using Lagrange multipliers [8]. The results are shown in Table I. Note that, for a given entropy, maximizing the disequilibrium is equivalent to minimizing the Tsallis entropy with parameter $q = 2$. Note also that for an isolated sys-

TABLE I: Probability values, f_j, that give a maximum of disequilibrium, D, or equivalently complexity, for a given entropy, H.

Number of states with f_j	f_j	Range of f_j
1	$f_{\max}$	$1/N \ \ldots\ 1$
$N-1$	$(1-f_{\max})/(N-1)$	$0 \ \ldots\ 1/N$

tem the entropy variable is equivalent to a streched time scale, due to its monotonic increase with time given by the second law of thermodynamics. The results of Table I, graphically represented in Fig. 3, show that the maximum complexity distribution can be split into two components. One of them consists of a background equiprobability distribution for all accessible states, which will be denoted as the "people distribution". The other one, with the remaining probability, comprises the particular state with the highest probability and is called the "king distribution". The final maximum complexity distribution is the sum of the people and the king distributions. When the system reaches the equilibrium, the king and people distributions merge leaving only the equiprobability distribution.

4. MAXIMUM COMPLEXITY DISTRIBUTION OF AN ISOLATED MONODIMENSIONAL IDEAL GAS

The derivation of a maximum complexity distribution will be based on the symmetry of the momentum phase space and on particular initial condition considerations. As an extension of the former discrete case given in Table I, the distribution we are looking for will have two components. The people distribution component will be the equiprobability distribution and the king distribution will be made by choosing a particular dominant state according to plausible arguments derived from the initial state of the system.

First, let us obtain by symmetry arguments how the functional dependence of the equilibrium distribution, or equivalently the equiprobabilty one, looks when only one variable is maintained and all the rest are integrated. In an isolated ideal gas with n particles, all accessible states lie on the surface of a hypersphere in the $\hat{p}_n$-momentum phase space. If the energy of a single particle is $e_i = \hat{p}_i^2/2$, then the total energy of the ensemble is $E = \sum_{i=1}^{n} e_i$. The mean energy per particle e will be $e = E/n$. If the gas is in equilibrium, the micro-

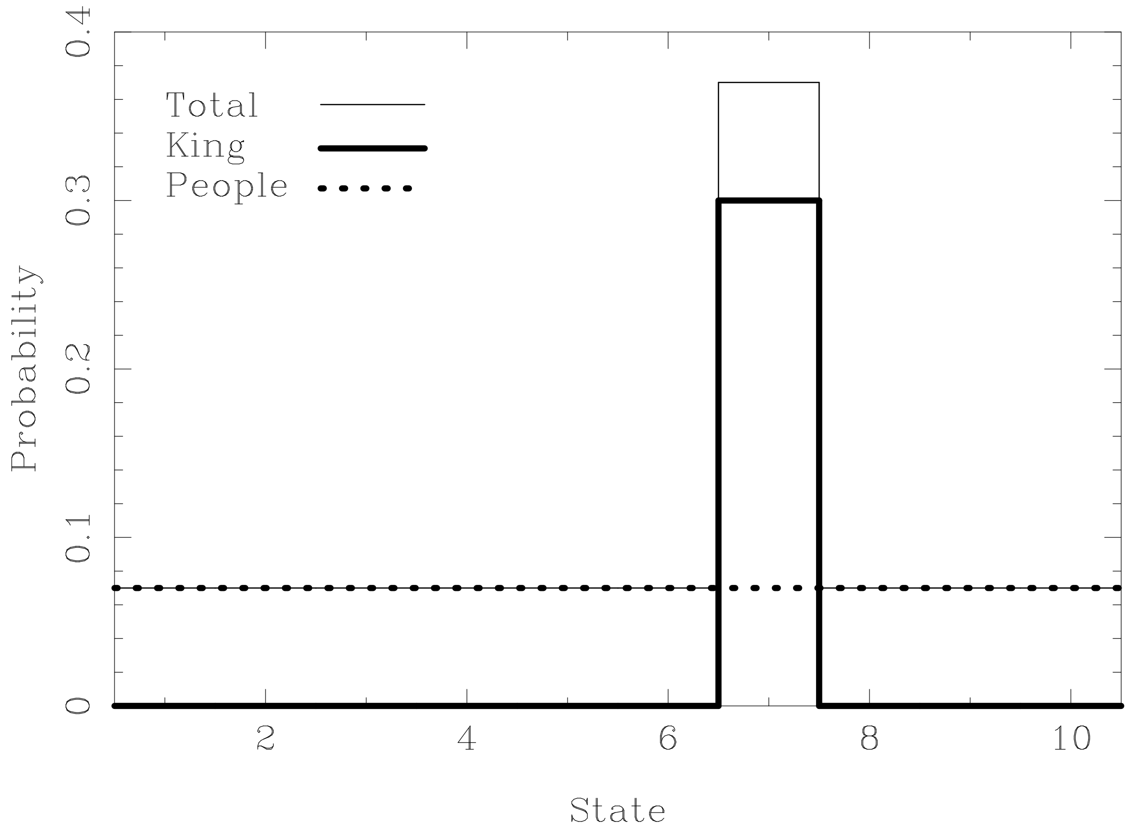

FIG. 3: Microcanonical maximum complexity distribution derived in Ref. [8] (thin solid line). It is the sum of the king (thick solid line) and the people, or equiprobability, distribution (dotted line).

canonical distribution, h, is the equiprobability for all accessible states, i.e., all points in phase space lying on the hypersphere surface have the same weight in the distribution h. This distribution is given by the expression

$$\begin{aligned} h(\theta_{n-1},\theta_{n-2},\ldots,\theta_1)d\theta_{n-1}d\theta_{n-2}\ldots d\theta_1 = \\ r^{n-1}d\theta_{n-1}\sin\theta_{n-1}d\theta_{n-2}\sin\theta_{n-1}\sin\theta_{n-2}d\theta_{n-3}\ldots \\ \sin\theta_{n-1}\sin\theta_{n-2}\ldots\sin\theta_2 d\theta_1, \end{aligned} \tag{3}$$

where the original phase space variables, $(\hat{p}_1,\hat{p}_2,\ldots,\hat{p}_n)$, have been converted to the spherical coordinates, $(r,\theta_1,\theta_2,\ldots,\theta_{n-1})$, with $r^2/2 = ne$. To obtain the one-particle momentum distribution of this system in equilibrium h can be integrated over all coordinates except θ_{n-1} obtaining the function g,

$$g(\theta_{n-1})d\theta_{n-1} = C' r^{n-1}\sin^{n-2}\theta_{n-1}d\theta_{n-1}, \tag{4}$$

where C' is the constant of integration. Converting this result back to the $\hat{p}_n$-momentum coordinate via the relation $\hat{p}_n = r\cos\theta_{n-1}$ we have the final distribution f,

$$f(\hat{p}_n)d\hat{p}_n = C' r^{n-2}\left(1 - \hat{p}_n^2/r^2\right)^{\frac{n-3}{2}} d\hat{p}_n. \tag{5}$$

Taking the limit for a large number, n, of particles the one-particle momentum distribution in equilibrium is obtained,

$$f_{EQ}(\hat{p}_n)d\hat{p}_n = C\exp(-\hat{p}_n^2/4e)d\hat{p}_n, \tag{6}$$

where $C = \sqrt{1/(4\pi e)}$ is the normalization constant. Substituting $e = KT/2$, K being the Boltzmann constant and T the temperature, the familiar one-particle ideal-gas momentum distribution is obtained, i.e., the Maxwell–Boltzmann distribution. It is remarkable that this result has been obtained in the microcanonical ensemble although this distribution is usually presented as a typical derivation from the canonical formalism. The people distribution, f_P, being an equiprobability distribution, its formal expression will be the same as the equilibrium one,

$$f_P(\hat{p}_n) = C_P\exp(-\hat{p}_n^2/4e_P). \tag{7}$$

Fig. 4 shows the people distribution in a dimensional space with just three particles as a dashed mesh surface.

Second, let us discuss how to find a king distribution for our system. In the scenario of injecting two extremely energetic particles into the gas in equilibrium, the states with the highest velocities will be populated with a certain number of particles in phase space. Using symmetry considerations, all high-velocity components in phase space for each one of those particles should be equivalent in this distribution. It then seems plausible to assume that the high-probability state of the king distribution can be formed by all the spherical caps in phase space centered on the maximum possible velocities for each particle. Fig. 4 illustrates this concept in a small dimensional space with just three particles. The king distribution in this phase space is shown as a mesh of solid lines: the probability of a state lying inside one of these caps is uniform and zero if it lies outside. Each of these caps is identified by the angle α shown in the figure. Integrating for all momentum dimensions except one, the one

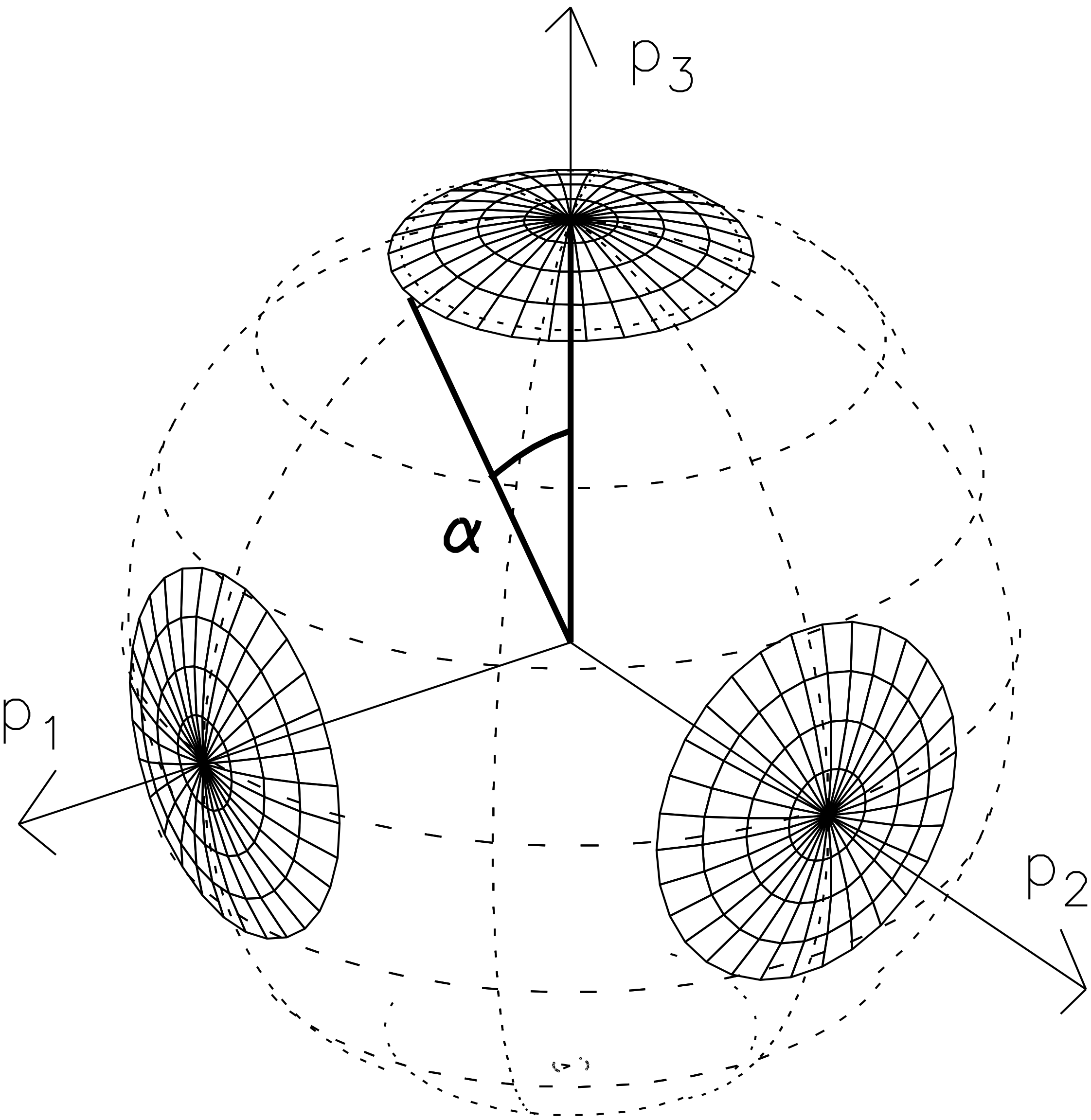

FIG. 4: Non-zero constant probability surfaces of the people (dashed mesh) and king (solid mesh) distributions on the space ($3D$ sphere) of accessible states of a three particle monodimensional ideal gas.

particle momentum distribution f_K is obtained,

$$f_K(\hat{p}_n) = \begin{cases} \Phi(\hat{p}_n) & \text{if } \hat{p}_n < r\sin\alpha, \\ 0 & \text{if } r\sin\alpha \leq \hat{p}_n < r\cos\alpha, \\ C_K\ \mathrm{e}^{(-\hat{p}_n^2/4e_K)} & \text{if } r\cos\alpha \leq \hat{p}_n, \end{cases} \tag{8}$$

Since the spherical caps that are over the $\hat{p}_n = 0$ point only cover a part of the hypersphere surface given by the set of points $(\hat{p}_1, \hat{p}_2, \ldots, \hat{p}_{n-1}, \hat{p}_n \simeq 0)$, the function $\Phi(\hat{p}_n)$ will satisfy,

$\Phi(\hat{p}_n) < C_K \exp(-\hat{p}_n^2/4e_K)$.

The final exact expression for the maximum complexity non-equilibrium distribution will be the sum of both distributions,

$$f_{MC}(\hat{p}_n) = f_K(\hat{p}_n) + f_P(\hat{p}_n). \tag{9}$$

We can simplify this equation by noting that, for the $\hat{p}_n < r\sin\alpha$ cases, $\Phi(\hat{p}_n) \ll f_P(\hat{p}_n)$, and that, for the $r\cos\alpha < \hat{p}_n$ cases, $f_P(\hat{p}_n) \ll f_K(\hat{p}_n)$.

As a first approximation, the maximum complexity non-equilibrium distribution is obtained:

$$f_{MC}(\hat{p}_n) \cong \begin{cases} C_P \exp(-\hat{p}_n^2/4e_P) & \text{if } \hat{p}_n < \hat{p}_0, \\ C_K \exp(-\hat{p}_n^2/4e_K) & \text{if } \hat{p}_0 \leq \hat{p}_n, \end{cases} \tag{10}$$

where the momentum $\hat{p}_0 \equiv r\cos\alpha$ is defined. Hence the final maximum complexity distribution is a two-component non-overlapping Gaussian function characterized by the parameters e_P and e_K, which vary with time when the system decays towards equilibrium, as seen in Fig. 1.

5. CONCLUSION

In conclusion, a maximum complexity one-particle momentum distribution has been derived for an isolated monodimensional ideal gas far from equilibrium. It is based on maximizing the disequilibrium, or equivalently minimizing the Tsallis entropy with parameter $q = 2$, for a given entropy, or equivalently time, in an isolated system. In a first approximation, the maximum complexity distribution is a double non-overlapping Gaussian distribution. Numerical simulations of a particular isolated monodimensional gas show, in clear agreement with our analytical result, a double Gaussian distribution when it decays towards equilibrium.

Acknowledgments

The figures in this paper have been prepared using the numerical programming language PDL (http://pdl.perl.org).

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